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1-[*N*-(*p*-Hydroxyphenyl)aminomethylidene]naphthalen-2(1*H*)-one propan-1-ol hemisolvate

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Key indicators

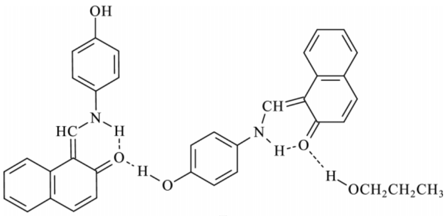
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.136
Data-to-parameter ratio = 17.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $2C_{17}H_{13}NO_2 \cdot C_3H_8O$, adopts the keto–amine tautomeric form, with strong intramolecular N—H···O and intermolecular O—H···O hydrogen bonds which form an almost planar two-dimensional network. The asymmetric unit contains two molecules of the Schiff base and one propan-1-ol solvent molecule.

Comment

2-Hydroxy Schiff base ligands and their complexes derived from the reaction of 2-hydroxy aromatic aldehydes with amines have been extensively studied. Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activities (Lozier *et al.*, 1975; Garnovskii *et al.*, 1993). Apart from their biological activity, photochromism and thermochromism are also characteristics of these materials, leading to their application in various areas, such as the control and measurement of radiation intensity, display systems and optical computers (Hadjoudis *et al.*, 1987; Yeap *et al.*, 2003). Two types of intramolecular hydrogen bonds (O—H···N and N—H···O) can exist in aldimine compounds derived from aromatic aldehydes having a hydroxyl group in an *ortho* position to the aldehyde group, and there is also tautomerism which accounts for the formation of either enol–imine or keto–amine tautomers (Gavranic *et al.*, 1996; Yıldız *et al.*, 1998; Odabaşoğlu, Albayrak, Büyükgüngör & Goesmann, 2003; Odabaşoğlu, Albayrak, Büyükgüngör & Lönnecke, 2003). In the field of coordination chemistry, this type of *ortho* hydroxylated Schiff bases has received considerable attention, particularly in the study of complex formation (Yeap *et al.*, 2003). This paper deals with the crystal structure of an interesting aromatic Schiff base ligand containing one naphthalene ring system.



(I)

Our previous crystallographic studies showed that an intramolecular N—H···O hydrogen bond exists in salicylaldimine derivatives in the solid state (Odabaşoğlu, Albayrak, Büyükgüngör & Goesmann, 2003) regardless of the nature of the group substituted on the aromatic ring. The N—H···O

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hydrogen bonds of (I) (Table 2) are also present in *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine (Kaitner & Pavlovic, 1996).

In (I), there are two symmetry-independent ligand molecules and one propan-1-ol molecule in the asymmetric unit (Fig. 1). Selected bond distances and bond angles of (I) are listed in Table 1. In the title compound, (I), the short C2—O1, C19—O3, C1—C11 and C18—C28 bonds can be considered as C=O and C=C double bonds, respectively. This fact, along with the very short C3—C4 and C20—C21 bonds, suggests the presence of a significant quinoidal effect. A similar quinoidal effect was observed for *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine (Kaitner & Pavlovic, 1996) and 1-[*N*-(4-methyl-2-pyridyl)aminomethylidene]naphthalen-2(1*H*)-one (Elerman *et al.*, 1998).

The study of Schiff bases has led to the proposal that molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar. This planarity of the molecule allows the proton to be transferred through the hydrogen bond in the ground state with a small energy requirement (Hadjoudis *et al.*, 1987). Our investigation shows that the ligand molecules of (I) are almost planar, with a dihedral angle of 6.66 (7)° between *A* (C1–C10) and *B* (C12–C17) and 6.89 (8)° between *C* (C18–C27) and *D* (C29–C34). The two independent naphthalene groups in the asymmetric unit of (I) form a dihedral angle of 4.91 (4)° and these naphthalene planes are almost perpendicular to the plane through propan-1-ol, the dihedral angles being 85.91 (1) for *A* and 85.1 (1)° for *C*.

Experimental

The title compound, (I), was prepared by refluxing a mixture of a solution containing 1.73 g (10 mmol) of 2-hydroxy-1-naphthaldehyde in 100 ml ethyl alcohol and a solution containing 1.09 g of *p*-hydroxyaniline (10 mmol) in 50 ml ethyl alcohol. The reaction mixture was stirred for 1.5 h under reflux. Microcrystals of (I) were obtained by allowing the clear solution to stand overnight. The powder product was dissolved and recrystallized from propan-1-ol solution (yield 95%; m.p. 605–607 K).

Crystal data

$2C_{17}H_{13}NO_2\cdot C_3H_8O$	$D_x = 1.292$ Mg m^{-3}
$M_r = 586.66$	Mo Kα radiation
Monoclinic, $P2_1/c$	Cell parameters from 11900 reflections
$a = 17.2090$ (17) Å	$\theta = 4.1$–$29.1°$
$b = 8.9038$ (6) Å	$\mu = 0.09$ mm^{-1}
$c = 19.9334$ (19) Å	$T = 293$ K
$\beta = 99.084$ (8)°	Rectangular, orange
$V = 3016.0$ (5) Å^3	0.55 × 0.32 × 0.15 mm
$Z = 4$	

Data collection

Stoe IPDS-2 diffractometer	$R_{\rm int} = 0.053$
ω rotation scans	$\theta_{\max} = 27.5°$
Absorption correction: none	$h = -21 \rightarrow 22$
24 465 measured reflections	$k = -11 \rightarrow 11$
6928 independent reflections	$l = -25 \rightarrow 25$
3578 reflections with $I > 2\sigma(I)$	

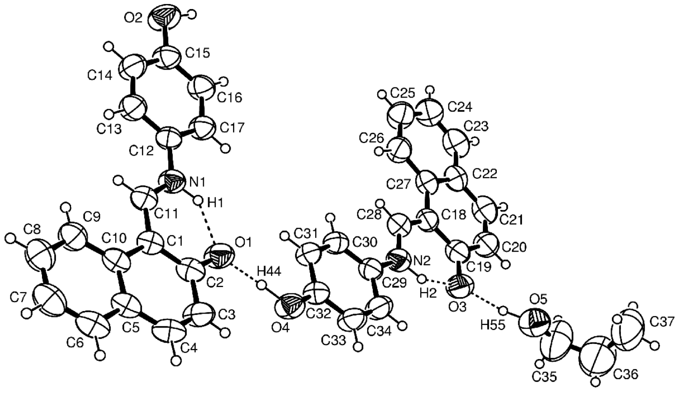

Figure 1
A view of the asymmetric unit of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0779P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.136$	$(\Delta/\sigma)_{\max} = 0.009$
$S = 0.88$	$\Delta\rho_{\max} = 0.36$ e Å^{-3}
6928 reflections	$\Delta\rho_{\min} = -0.24$ e Å^{-3}
405 parameters	

Table 1
Selected geometric parameters (Å, °).

C1—C11	1.399 (2)	C18—C28	1.397 (2)
C1—C2	1.423 (2)	C18—C19	1.429 (2)
C1—C10	1.451 (2)	C18—C27	1.454 (2)
C2—O1	1.2950 (19)	C19—O3	1.292 (2)
C2—C3	1.431 (2)	C19—C20	1.422 (2)
C3—C4	1.343 (2)	C20—C21	1.341 (2)
C4—C5	1.422 (3)	C21—C22	1.425 (3)
C5—C10	1.406 (2)	C22—C27	1.402 (2)
C12—N1	1.416 (2)	C29—N2	1.408 (2)
C11—C1—C2	119.30 (15)	C28—C18—C27	121.00 (17)
C11—C1—C10	120.79 (16)	O3—C19—C20	119.82 (18)
O1—C2—C1	121.81 (14)	O3—C19—C18	121.51 (16)
O1—C2—C3	119.66 (17)	N2—C28—C18	122.99 (17)
N1—C11—C1	124.12 (17)	C11—N1—C12	127.69 (17)
C28—C18—C19	119.65 (16)	C28—N2—C29	127.75 (17)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.95 (2)	1.79 (2)	2.556 (2)	136 (2)
N2—H2···O3	0.97 (2)	1.68 (2)	2.539 (2)	145 (2)
O2—H22···O4$^{\rm i}$	0.82	1.89	2.701 (2)	168
O4—H44···O1	0.82	1.74	2.552 (2)	169
O5—H55···O3	0.82	1.94	2.749 (2)	170

Symmetry code: (i) $x, \frac{3}{2} - y, z - \frac{1}{2}$.

Except for those attached to N atoms, which were freely refined, all H atoms were treated using a riding model, with a C—H distance of 0.93 Å for aromatic H atoms, 0.96 Å for methyl H atoms and 0.97 Å for methylene H atoms, and an O—H distance of 0.82 Å. The $U_{\rm iso}$ values for these H atoms were assigned as $1.2U_{\rm eq}$ of the parent atom.

The anisotropic displacement parameters of atoms C35, C36 and C37 are rather high, indicating that there is some unresolved disorder.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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